C11	0.8255 (2)	0.5446 (2)	0.7326 (2)	0.039
C12	0.8468 (2)	0.4821 (2)	0.6675 (2)	0.038
C13	0.8506 (2)	0.6388 (2)	0.7325 (2)	0.044
C14	0.9174 (3)	0.7543 (3)	0.8191 (3)	0.068
C15	0.9078 (4)	0.7881 (4)	0.9175 (5)	0.125
C16	0.9912 (3)	0.7626 (4)	0.7684 (5)	0.118
C17	0.9111 (2)	0.4910 (2)	0.5927 (2)	0.038

Table 2. *Selected geometric parameters* (Å, °)

C1—C2	1.396 (6)	C9—C9a	1.519 (5)
C1—C9a	1.381 (5)	C9—C11	1.537 (4)
C2—C3	1.376 (6)	C10—C10a	1.536 (4)
C3—C4	1.392 (5)	C10—C12	1.533 (4)
C4—C4a	1.374 (5)	C11—C12	1.329 (4)
C4a—C9a	1.393 (4)	C11—C13	1.483 (4)
C4a—C10	1.513 (4)	C12—C17	1.474 (4)
C5—C6	1.396 (6)	C14—C15	1.413 (8)
C5—C10a	1.371 (5)	C14—C16	1.416 (7)
C6—C7	1.398 (7)	C13—O1	1.323 (4)
C7—C8	1.374 (7)	C13—O2	1.203 (4)
C8—C8a	1.361 (5)	C14—O1	1.474 (3)
C8a—C9	1.532 (5)	C17—O3	1.285 (3)
C8a—C10a	1.395 (4)	C17—O4	1.246 (3)
C2—C1—C9a	118.9 (4)	C4a—C10—C12	106.3 (2)
C1—C2—C3	120.6 (4)	C10a—C10—C12	105.3 (2)
C2—C3—C4	120.2 (4)	C5—C10a—C8a	120.6 (3)
C3—C4—C4a	119.5 (4)	C5—C10a—C10	126.8 (3)
C4—C4a—C9a	120.4 (3)	C8a—C10a—C10	112.6 (3)
C4—C4a—C10	127.0 (3)	C9—C11—C12	113.6 (3)
C9a—C4a—C10	112.6 (3)	C9—C11—C13	118.5 (2)
C6—C5—C10a	119.0 (4)	C12—C11—C13	127.1 (3)
C5—C6—C7	119.9 (4)	C10—C12—C11	114.3 (3)
C6—C7—C8	119.9 (4)	C10—C12—C17	120.9 (2)
C7—C8—C8a	120.3 (4)	C11—C12—C17	124.9 (3)
C8—C8a—C9	127.1 (3)	C11—C13—O1	113.0 (3)
C8—C8a—C10a	120.3 (3)	C11—C13—O2	122.2 (3)
C9—C8a—C10a	112.7 (3)	O1—C13—O2	124.7 (3)
C8a—C9—C9a	105.5 (2)	O1—C14—C15	110.4 (4)
C8a—C9—C11	104.6 (2)	O1—C14—C16	109.3 (4)
C9a—C9—C11	106.3 (2)	C15—C14—C16	120.6 (5)
C1—C9a—C4a	120.4 (3)	C12—C17—O3	117.1 (3)
C1—C9a—C9	126.3 (3)	C12—C17—O4	120.2 (3)
C4a—C9a—C9	113.3 (3)	O3—C17—O4	122.7 (3)
C4a—C10—C10a	105.2 (2)	C13—O1—C14	115.8 (3)

The structure was determined by direct methods. There is minor disorder in the isopropyl group; this was modelled by a split C16 site [15% occupancy (not refined) for C16′ at 1.014 (1), 0.725 (1), 0.897(2), isotropic], but the geometry of the group as a whole is rather unsatisfactory. Data collection, cell refinement, data reduction, structure solution, structure refinement and molecular graphics: *TEXSAN* (Molecular Structure Corporation, 1990).

We thank the Natural Sciences and Engineering Research Council of Canada for financial support.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry and stereo molecular and packing diagrams have been deposited with the IUCr (Reference: BK1006). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Molecules Isoelectronic with Triphenylmethanol: Diphenyl(4-pyridyl)methanol and Triphenylmethylamine

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Abstract

Diphenyl(4-pyridyl)methanol, $C_{18}H_{15}NO$, forms chains in the solid state in which the molecules are linked by O—H···N hydrogen bonds; the O atoms, although potential hydrogen-bond acceptors, are not utilized as such in the intermolecular hydrogen bonding. Triphenylmethylamine, $C_{19}H_{17}N$, crystallizes as isolated molecules with perfectly ordered pyramidal NH_2 groups; there is no intermolecular hydrogen bonding despite the availability of potential hydrogen-bond donors and acceptors.

Comment

Triphenylmethanol crystallizes as almost perfectly tetrahedral tetramers, with the four hydroxyl H atoms presumably disordered over the six O···O edges (Ferguson, Gallagher, Glidewell, Low & Scrimgeour, 1992). Despite the exact match of the number of hydrogen-bond donors and hydrogen-bond acceptors in this tetrameric system, a structure is adopted which cannot have one O—H···O hydrogen bond per O···O atom pair. With only modest changes in the steric demands at the unique central C atom, while keeping the number of hydrogen-bond donors and acceptors unchanged, the patterns of hydrogen bonding can be altered drastically. Thus in 1,1,2-triphenylethanol there is O—H···π(arene), rather than O—H···O, intermolecular hydrogen bonding (Ferguson, Gallagher, Glidewell & Zakaria, 1994), while the crystal structures of 1,2,3-triphenyl-2-propanol and tribenzylmethanol contain no hydrogen bonds at all (Ferguson, Gallagher, Glidewell, Liles & Zakaria, 1993).

Etter has formulated some general principles for hydrogen-bond formation in systems where the numbers of hydrogen-bond donors and acceptors are identical (Etter, 1990; Etter, McDonald & Bernstein, 1990; Etter & Reutzel, 1991). Where there is an excess of hydrogen-bond donors over acceptors, the numerical mis-

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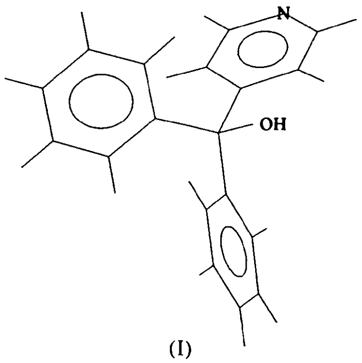
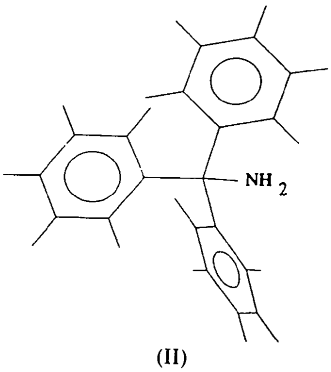
match can often be accommodated either by formation of *X*—H···π(arene) hydrogen bonds or by a change in hybridization at the acceptor site (Hanton, Hunter & Purvis, 1992); on the other hand, an excess of acceptors, *X*, can sometimes be accommodated by formation of C—H···*X* hydrogen bonds involving weakly acidic C—H bonds on benzenoid rings as the hydrogen-bond donors (Hunter, 1991).

As a test of these ideas for cases of numerical mismatch between hydrogen-bond donors and acceptors, we report here the structures of two isoelectronic analogues of triphenylmethanol designed to produce the minimum changes in the steric requirements at the central C atom. In diphenyl(4-pyridyl)methanol, (I), there is an excess of conventional hydrogen-bond acceptors over donors, whereas in triphenylmethylamine, (II), there is an excess of donors over acceptors. In contrast to the previous findings (Hunter, 1991; Hanton, Hunter & Purvis, 1992), compound (I) employs only one of its two possible acceptor sites in hydrogen-bond formation, while compound (II) forms no hydrogen bonds at all.



(I)



(II)

Compound (I) forms chains in the solid state in which the molecules are linked by O—H···N hydrogen bonds (Fig. 1). These chains lie parallel to the *a* axis and the space-group symmetry demands two sets of antiparallel chains: viewed in the *ab* plane, the sequence of the chain directions is up, up, down, down, while viewed in the *ac* plane the sequence is up, down, up, down. Each molecule uses a single hydrogen-bond acceptor: the N atom of the 4-pyridyl group, in preference to the O atom presumably because the N atom is both the more basic acceptor and the less sterically hindered acceptor. The excess acceptor is not incorporated into the hydrogen-bonding scheme. In this respect, the hydrogen-bonding scheme is similar to that in the crystal structure of 3-(diphenylhydroxymethyl)-3*H*-azepine (Lindner & von Gross, 1973).

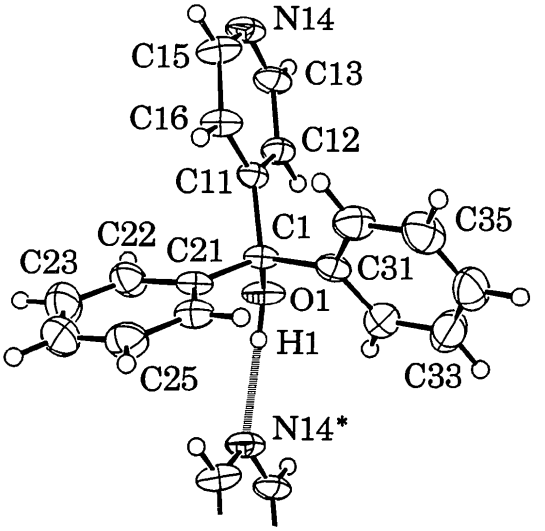


Fig. 1. A view of molecule (I) and an O—H···N hydrogen bond to an adjacent molecule (1 + *x*, *y*, *z*), with our numbering scheme; non-H atoms are shown with displacement ellipsoids drawn at the 30% probability level and all H atoms are drawn as small spheres of arbitrary size.

Within the molecules of (I), the C—O distance is 1.419 (6) Å, less than the lower quartile value of 1.424 Å for alcohols (Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987), and the range and mean of the C_{sp^3}—C(aryl) distances are 1.527 (7)-1.535 (7) Å and 1.532 Å (higher than the upper quartile value of 1.521 Å), respectively. The other intramolecular distances are unexceptional, *e.g.* the aromatic C—C distances are in the range 1.362 (10)-1.393 (7) Å, with a mean value of 1.378 (10) Å. For the O—H···N hydrogen bonds, the O···N distance is 2.861 (6) Å, indicative of fairly weak hydrogen bonding, with an O—H···N angle 176 (5)°.

The structure of compound (II) consists of isolated molecules (Fig. 2); the C—N distance is 1.481 (3) Å (slightly above the upper quartile value of 1.476 Å for primary amines) and the C_{sp^3}—C(aryl) distances are essentially identical in the range 1.539 (3)-1.541 (3) Å, again somewhat above the upper quartile value of 1.521 Å, and significantly longer than the corresponding distances in triphenylmethanol [range 1.509 (14)-1.522 (10) Å, mean 1.514 Å (Ferguson, Gallagher, Glidewell, Low & Scrimgeour, 1992)]. The aromatic C—C distances are in the range 1.357 (5)-1.398 (3) Å, with a mean value of 1.382 (9) Å. The bond lengths around the central C atom

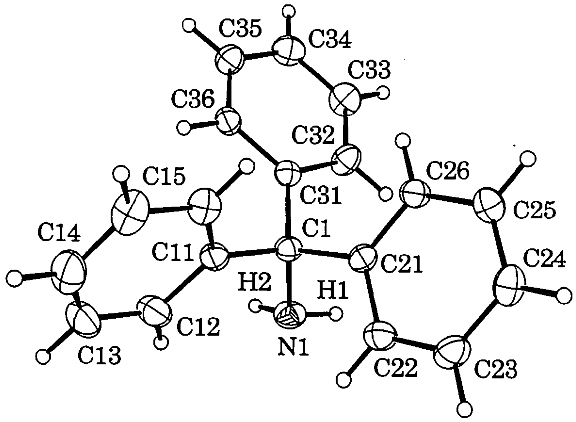


Fig. 2. A view of molecule (II) with our numbering scheme; non-H atoms are shown with displacement ellipsoids drawn at the 30% probability level and all H atoms are drawn as small spheres of arbitrary size.

in (II) suggest the possibility that the NH_2 group in (II) is slightly more sterically demanding than the OH group in triphenylmethanol, although this does not fully explain the complete lack of hydrogen bonding in (II). There is no indication that the amino H atoms take part in any hydrogen bonding; the shortest intermolecular contacts H1···C15 [at $2 - x, -\frac{1}{2} + y, \frac{1}{2} + z$; 2.80 (3) Å] and H2···C35 [at $-1 + x, y, z$; 2.82 (3) Å] are too long even for weak H···π(arene) interactions.

The conformation of (II) is such that there is almost perfect staggering of the fully ordered N—H bonds and the C1—C*n*1 bonds (where $n = 1, 2$ or 3). Because of the propeller-like twist of the phenyl rings about the C_{sp^3}—C(aryl) bond [the dihedral angles N1—C1—C*n*1—C*n*2 are −12.0 (1), −47.2 (2), −60.3 (2)°, for $n = 1, 2$ and 3, respectively], the molecules can have no symmetry if the pyramidal NH_2 group is ordered and static; hence the observation of the chiral space group $P2_12_12_1$ is not unusual even though, in solution, the molecular structure of (II) is averaged to an achiral configuration.

In triphenylmethanethiol, Ph_3CSH, a precise analogue of triphenylmethanol, there is no hydrogen bonding at all and the closest S···S distance is 4.653 Å (Bernardinelli, Geoffroy & Franzi, 1991). Other close analogues which have been structurally characterized include Ph_3CCl (Dunand & Gerdil, 1982) and Ph_3CBr (Dunand & Gerdil, 1984), in which the molecules are stacked in a head-to-head arrangement along crystallographic threefold axes, with *X*···*X* (*X* = Cl, Br) distances being significantly shorter than the sum of van der Waals radii. Ph_3CF has been characterized in a mixed crystal with phenyltropylium tetrafluoroborate (Takusagawa, Jacobson, Trahanovsky & Robbins, 1976).

Experimental

Crystals of compounds (I) and (II) were obtained by recrystallization from ethanol and dichloromethane solutions, respectively.

Compound (I)

Crystal data

$C_{18}H_{15}NO$
$M_r = 261.32$
Monoclinic
$P2_1/c$
$a = 7.7221$ (8) Å
$b = 14.9146$ (20) Å
$c = 11.8191$ (14) Å
$\beta = 95.351$ (9)°
$V = 1355.3$ (3) Å^3
$Z = 4$
$D_x = 1.281$ Mg m^{-3}

Mo *Kα* radiation
$\lambda = 0.7107$ Å
Cell parameters from 25 reflections
$\theta = 10.50$–18.00°
$\mu = 0.07$ mm^{-1}
$T = 293$ K
Plate
0.05 × 0.25 × 0.47 mm
Colourless

Data collection

Enraf-Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
2546 measured reflections
2368 independent reflections
1011 observed reflections [$I > 3.0\sigma(I)$]

$R_{\rm int} = 0.018$
$\theta_{\rm max} = 24.92°$
$h = -9 \rightarrow 9$
$k = 0 \rightarrow 17$
$l = 0 \rightarrow 14$
3 standard reflections
frequency: 60 min
intensity variation: 1.0%

Refinement

Refinement on *F*
$R = 0.043$
$wR = 0.049$
$S = 1.19$
1011 reflections
186 parameters
$w = 1/[\sigma^2(F) + 0.0008F^2]$
$(\Delta/\sigma)_{\rm max} = 0.002$
$\Delta\rho_{\rm max} = 0.17$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.19$ e Å^{-3}

Extinction correction: Larson (1970)
Extinction coefficient: 0.22 (14) × 10^4
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for compound* (I)

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
O1	0.7084 (5)	0.5400 (3)	0.1399 (3)	0.0398 (24)
C1	0.6346 (6)	0.5360 (3)	0.2454 (4)	0.029 (3)
C11	0.4381 (6)	0.5254 (3)	0.2157 (4)	0.028 (3)
C12	0.3584 (6)	0.5588 (3)	0.1137 (4)	0.035 (3)
C13	0.1804 (7)	0.5520 (4)	0.0927 (4)	0.041 (3)
N14	0.0778 (5)	0.5166 (3)	0.1643 (4)	0.042 (3)
C15	0.1545 (7)	0.4829 (4)	0.2609 (5)	0.046 (4)
C16	0.3320 (7)	0.4860 (4)	0.2882 (4)	0.040 (3)
C21	0.7058 (6)	0.4530 (4)	0.3096 (4)	0.032 (3)
C22	0.6904 (7)	0.3708 (4)	0.2546 (5)	0.046 (3)
C23	0.7560 (9)	0.2939 (4)	0.3061 (5)	0.062 (4)
C24	0.8415 (8)	0.2969 (4)	0.4145 (5)	0.058 (4)
C25	0.8555 (7)	0.3769 (4)	0.4701 (5)	0.049 (3)
C26	0.7899 (7)	0.4546 (4)	0.4190 (4)	0.038 (3)
C31	0.6685 (7)	0.6234 (3)	0.3124 (4)	0.032 (3)
C32	0.7891 (7)	0.6850 (4)	0.2814 (4)	0.044 (3)
C33	0.8206 (8)	0.7628 (4)	0.3426 (6)	0.056 (4)
C34	0.7324 (9)	0.7823 (4)	0.4336 (5)	0.057 (4)
C35	0.6113 (8)	0.7233 (5)	0.4661 (5)	0.056 (4)
C36	0.5801 (7)	0.6448 (4)	0.4056 (5)	0.047 (3)

Table 2. *Selected geometric parameters* (Å, °) *for compound* (I)

O1—C1	1.419 (6)	C1—C31	1.535 (7)
O1—H1	0.89 (6)	C13—N14	1.322 (8)
C1—C11	1.534 (6)	N14—C15	1.334 (7)
C1—C21	1.527 (7)		
C1—O1—H1	110 (3)	C1—C11—C12	120.6 (4)
O1—C1—C11	105.9 (4)	C1—C11—C16	122.5 (4)
O1—C1—C21	108.4 (4)	C1—C21—C22	118.2 (4)
O1—C1—C31	110.8 (4)	C1—C21—C26	124.2 (5)
C11—C1—C21	109.5 (4)	C1—C31—C32	121.0 (5)
C11—C1—C31	108.8 (4)	C1—C31—C36	122.2 (5)
C21—C1—C31	113.3 (4)	O1—H1···N14^{i}	176 (5)
H1—O1—C1—C11	−167 (4)	O1—C1—C11—C12	−27.8 (3)
H1—O1—C1—C21	−50 (4)	O1—C1—C21—C22	−53.4 (4)
H1—O1—C1—C31	75 (4)	O1—C1—C31—C32	−13.7 (3)

Symmetry code: (i) $1 + x, y, z$.

Compound (II)

Crystal data

$C_{19}H_{17}N$
$M_r = 259.35$
Orthorhombic
$P2_12_12_1$
$a = 6.0541\ (5)$ Å
$b = 13.4943\ (13)$ Å
$c = 17.6027\ (23)$ Å
$V = 1438.1\ (3)$ Å^3
$Z = 4$
$D_x = 1.198$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 25 reflections
$\theta = 13.50\text{–}25.00°$
$\mu = 0.06$ mm^{-1}
$T = 293$ K
Block
0.60 × 0.35 × 0.20 mm
Colourless

Data collection

Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
1821 measured reflections
1821 independent reflections
1358 observed reflections [$I > 3.0\sigma(I)$]

$\theta_{\max} = 26.87°$
$h = 0 \rightarrow 7$
$k = 0 \rightarrow 17$
$l = 0 \rightarrow 22$
3 standard reflections frequency: 60 min intensity variation: < 1.0%

Refinement

Refinement on F
$R = 0.029$
$wR = 0.044$
$S = 1.19$
1358 reflections
190 parameters
$w = 1/[\sigma^2(F) + 0.0010F^2]$
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.12$ e Å^{-3}

Extinction correction: Larson (1970)
Extinction coefficient: 1.4 (3) × 10^4
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for compound* (II)

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
N1	0.8531 (3)	0.84285 (16)	0.20549 (13)	0.0483 (11)
C1	1.0746 (3)	0.88933 (15)	0.20452 (11)	0.0358 (9)
C11	1.0554 (3)	0.99269 (15)	0.16810 (10)	0.0382 (9)
C12	0.8676 (4)	1.02351 (19)	0.12976 (15)	0.0568 (13)
C13	0.8553 (5)	1.11751 (23)	0.09868 (16)	0.0702 (17)
C14	1.0252 (6)	1.18248 (19)	0.10579 (15)	0.0689 (17)
C15	1.2140 (6)	1.15375 (17)	0.14330 (14)	0.0610 (15)
C16	1.2285 (4)	1.05922 (15)	0.17432 (12)	0.0491 (11)
C21	1.1400 (3)	0.90519 (14)	0.28826 (11)	0.0358 (9)
C22	0.9858 (4)	0.94739 (17)	0.33657 (12)	0.0479 (11)
C23	1.0335 (5)	0.96423 (19)	0.41229 (13)	0.0534 (12)
C24	1.2383 (5)	0.93837 (15)	0.44080 (12)	0.0502 (12)
C25	1.3941 (4)	0.89843 (17)	0.39335 (13)	0.0481 (11)
C26	1.3475 (3)	0.88288 (16)	0.31675 (12)	0.0410 (10)
C31	1.2379 (3)	0.82236 (13)	0.16127 (11)	0.0352 (9)
C32	1.2770 (4)	0.72636 (16)	0.18796 (12)	0.0484 (11)
C33	1.4158 (5)	0.66247 (16)	0.14942 (14)	0.0541 (13)
C34	1.5147 (4)	0.69141 (18)	0.08262 (14)	0.0524 (12)
C35	1.4765 (4)	0.78477 (17)	0.05495 (12)	0.0484 (12)
C36	1.3403 (4)	0.84998 (15)	0.09412 (11)	0.0395 (9)

Table 4. *Selected geometric parameters* (Å, °) *for compound* (II)

N1—C1	1.481 (3)	C1—C11	1.539 (3)
N1—H1	0.96 (3)	C1—C21	1.541 (3)
N1—H2	0.88 (3)	C1—C31	1.541 (3)
C1—N1—H1	108.6 (17)	C21—C1—C31	112.91 (16)
C1—N1—H2	108.1 (18)	C1—C11—C12	122.47 (20)
H1—N1—H2	107.0 (24)	C1—C11—C16	119.83 (18)
N1—C1—C11	108.66 (17)	C1—C21—C22	118.10 (18)
N1—C1—C21	106.29 (16)	C1—C21—C26	123.29 (17)
N1—C1—C31	109.78 (16)	C1—C31—C32	119.08 (18)
C11—C1—C21	106.98 (15)	C1—C31—C36	123.41 (17)
C11—C1—C31	111.98 (16)		
H1—N1—C1—C11	−170 (2)	N1—C1—C21—C22	−47.2 (2)
H2—N1—C1—C21	−171 (2)	N1—C1—C21—C26	135.4 (2)
N1—C1—C11—C12	−12.0 (1)	N1—C1—C31—C32	−60.3 (2)
N1—C1—C11—C16	166.8 (3)	N1—C1—C31—C36	115.9 (2)

The space groups for (I) and (II) were determined unambiguously from the systematic absences [for (I), $P2_1/c$, $h0l$ absent if $l = 2n + 1$, $0k0$ absent if $k = 2n + 1$; for (II), $P2_12_12_1$, $h00$ absent if $h = 2n + 1$, $0k0$ absent if $k = 2n + 1$, $00l$ absent if $l = 2n + 1$]. All H atoms were clearly visible in difference maps at intermediate stages of the refinement. All C—H H atoms were positioned on geometric grounds (C—H = 0.95 Å) and included as riding atoms in the structure-factor calculations. In (I), the hydroxyl H atom, and in (II), the two H atoms bonded to the N atom were allowed to refine isotropically. Molecule (II) occurs in a chiral space group, but the data did not allow us to determine which enantiomer was in the data crystal as there was no significant difference between the R factor of the model reported here and that of its enantiomer (Rogers, 1981). There is no solvent of crystallization present in the lattices and an examination of the crystal structure using *PLATON* (Spek, 1990) revealed no potential volume for any solvent molecules. Data collection and cell refinement were performed using *CAD-4 Software* (Enraf-Nonius, 1989). Data reduction, structure solution and refinement, and preparation of the material for publication were performed using *NRCVAX* (Gabe, Le Page, Charland, Lee & White, 1989). The displacement-ellipsoid diagrams were prepared using *ORTEP*II (Johnson, 1976).

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Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: HA1086). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2,2,2-Triphenylethanol: a Hydrogen-Bonded Tetramer Based upon a Centrosymmetric $R_4^4(8)$ Motif

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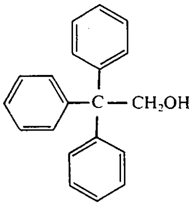
Abstract

2,2,2-Triphenylethanol, $C_{20}H_{18}O$, crystallizes as hydrogen-bonded tetrameric aggregates which are centrosymmetric. The resulting planar O_4 ring is almost square with O···O distances of 2.786 (2) and 2.822 (2) Å; the hydroxyl H atoms are fully ordered, one along each O···O edge of the O_4 parallelogram

Comment

The crystal structures of sterically congested monoalcohols display a wide variety of hydrogen-bonding patterns. The compounds Ph_3MOH (M = C, Si, Ge) all crystallize as hydrogen-bonded tetramers but while Ph_3COH forms an almost perfectly tetrahedral tetramer (Ferguson, Gallagher, Glidewell, Low & Scrimgeour, 1992), the tetramers of both Ph_3SiOH (Puff, Braun & Reuter, 1991) and Ph_3GeOH (Ferguson, Gallagher, Murphy, Spalding, Glidewell & Holden, 1992) contain puckered O-atom rings of approximate $\bar{4}$ (S_4) symmetry; $Ph_2(C_2H_5)COH$ forms similar $\bar{4}$ tetramers (Sultanov, Shnulin & Mamedov, 1985*a*). Although the dimers of Ph_2(ferrocenyl)COH are formed by O—H···O hydrogen bonds giving four-membered OHOH rings (Ferguson, Gallagher, Glidewell & Zakaria, 1993*a*), by contrast, in $Ph_2(PhCH_2)COH$ the sole intermolecular interactions leading to dimer formation are O—H···π(arene) hydrogen bonds (Ferguson, Gallagher, Glidewell & Zakaria, 1994), while the dimers of $Ph_2(PhCHF)COH$ depend upon O—H···F hydrogen bonds (DesMarteau, Xu & Witz, 1992). The structure of $Ph_2(CH_3)COH$ also contains O—H···π(arene) interactions, but these are intramolecular and the compound is monomeric (Sultanov, Shnulin & Mamedov, 1985*b*). In contrast to both Ph_3COH and $Ph_2(PhCH_2)COH$, the introduction of further methylene spacer groups between the phenyl rings and the quaternary C atom in $Ph(PhCH_2)_2COH$ and $(PhCH_2)_3COH$ leads to structures which contain no hydrogen bonds (Ferguson, Gallagher, Glidewell & Zakaria, 1993*b*). We have now extended the series $Ph_x(PhCH_2)_{3-x}COH$ to 2,2,2-triphenylethanol, $Ph_3C—CH_2—OH$ (I), in which the methylene spacer group has been placed between the quaternary C atom and the hydroxyl group; the structure of this compound shows yet another hydrogen-bonding pattern.



(I)

In the structure of 2,2,2-triphenylethanol there are two molecules, labelled A and B, in the asymmetric unit; these two molecules, together with a similar pair of molecules related to them by a centre of inversion, form a hydrogen-bonded tetrameric array (see Figs. 1 and 2). The centrosymmetry requires that all four O atoms in the tetramer are coplanar. The closest O···O distances are 2.786 (2)